



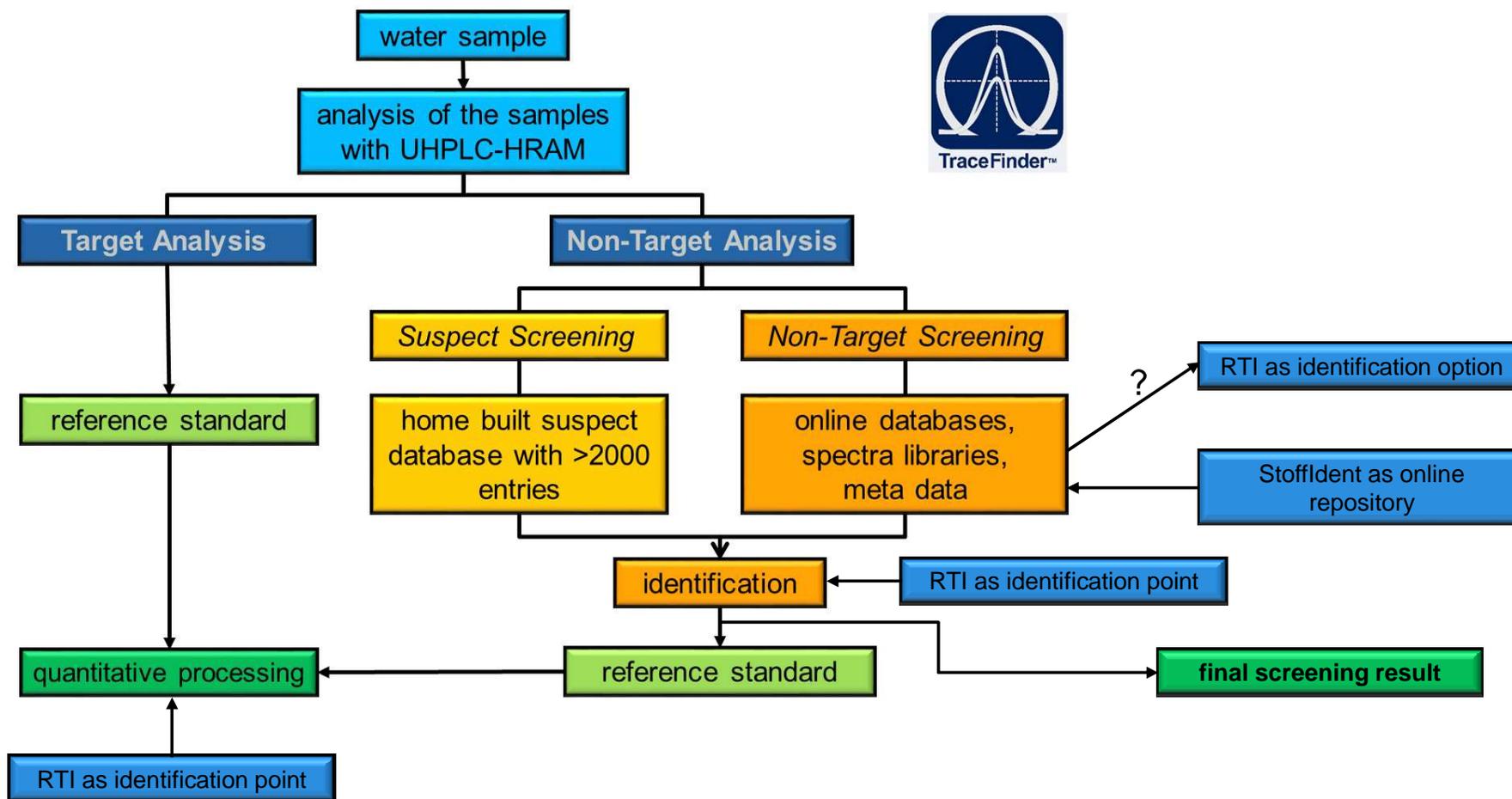
ThermoFisher
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ForIdent Workshop Langenau – Water Sample Screening Workflow

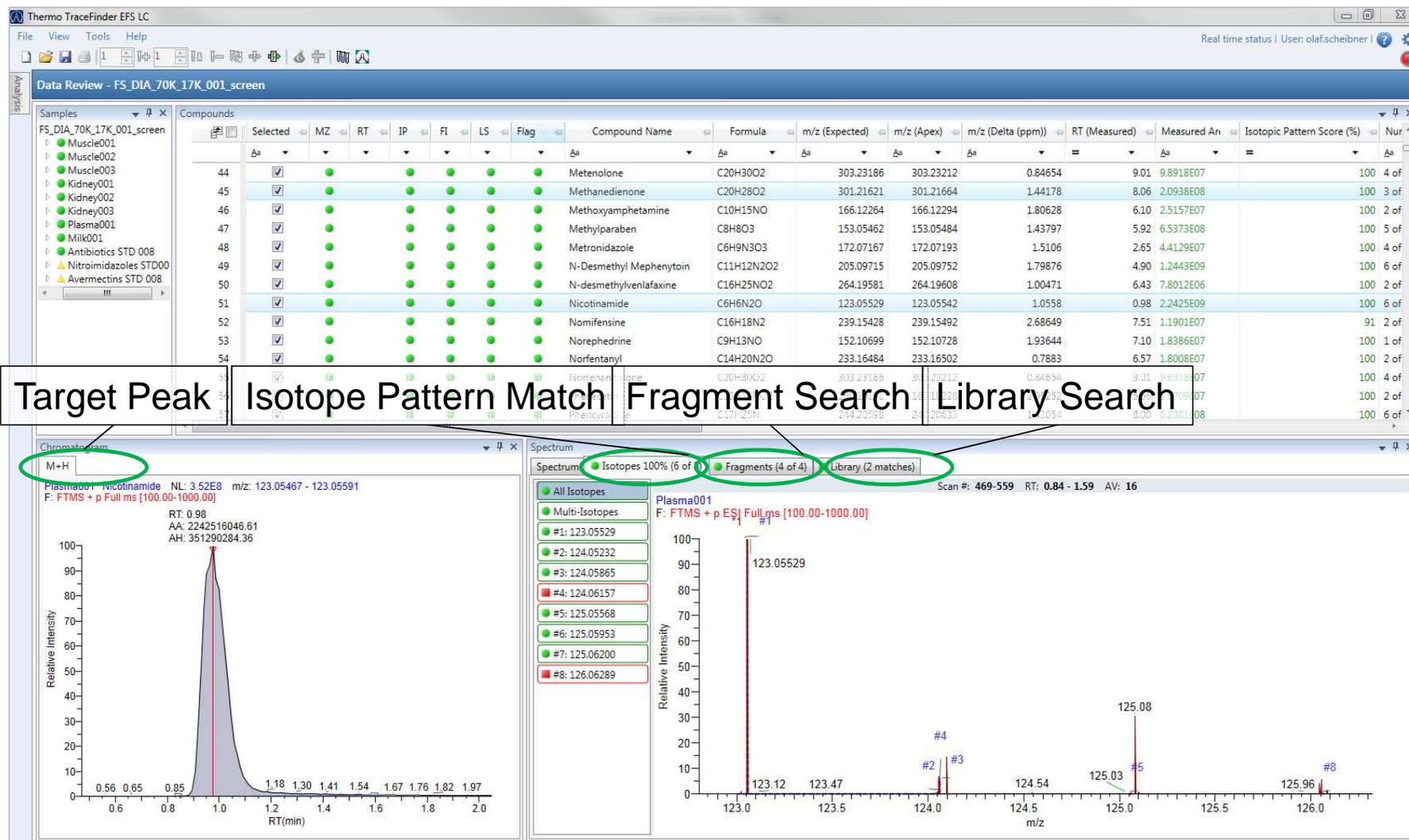
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(Slides contributed from Olaf Scheibner, Ryo Komatsuzaki)

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Quantitative and (Unknown) Screening Workflow



Result table for suspect screening (“final screening result”)



Biologics New Peak Detection

- Non-Targeted MS Peak Detection via Differential Analysis
- Brand new category

Process and status dependent labels

Processing parameters for new peak detection

XIC Differential Plot (Frame Plot)

Frame list with filter mechanism (hidden)

- Differential ratio threshold
- Root component for multi-isotope peaks
- Observed m/z
- Other fields available to display

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	
1	Frame ID	Component ID	Mass m/z	RT min	Ratio	Base Component	PR Element	PR Root	PR Size	Charge	Molecular Weight m/z																					
2	305	394	496.2670	11.06	1.352	4138	394	0	305	3	2	990.55948																				
3	449	647	613.3166	10.17	57.38	6936	647	0	449	3	2	1224.61911																				
4	459	504	422.7365	13.48	#####	#####	504	0	459	3	2	843.45841																				
5	466	362	498.8020	34.36	#####	#####	362	0	466	3	2	995.55945																				
6	595	590	745.3920	29.39	#####	#####	590	0	595	3	2	1489.76951																				
7	595	590	745.3920	29.39	#####	#####	590	0	595	3	2	1489.76951																				
8	658	610	773.8953	21.82	5.224	4652	610	0	658	3	2	1545.27610																				
9	659	607	695.8325	16.11	1684	4376	607	0	659	3	2	1389.65022																				
10	970	746	493.7696	9.72	2441	10486	746	0	970	2	2	985.62214																				
11	1568	874	558.3264	28.74	815	3378	874	0	1568	2	2	1114.63816																				
12	1633	781	573.3027	36.14	154	6261	781	0	1633	2	2	1144.93092																				
13	1862	634	337.2279	13.30	1047	1933	634	0	1862	1	2	672.44130																				
14	1879	1003	573.7949	42.60	3645	3593	1003	0	1879	2	2	1145.57517																				
15	2010	870	301.1914	13.30	218	1207	870	0	2010	1	3	900.55248																				
16	2193	1090	690.3795	41.13	3114	1586	1090	0	2193	2	2	1359.73252																				
17	3212	1163	451.2635	13.30	1732	9059	1163	0	3212	1	2	900.55240																				

Biologics New Peak Detection

- Non-Targeted MS Peak Detection
- Report Variable, Plot, and Table extensions

Frame ID	Mass m/z	RT min	Ratio	PR Element	PR Root	PR Size
15	284.1193	2.37	6.01	0	15	1
16	285.0789	2.84	6.42	0	16	1
28	333.0797	2.63	6.54	0	28	1
36	271.0632	2.70	6.47	0	36	1
40	252.1132	1.92	6.52	0	40	1
42	301.0735	2.70	5.54	0	42	1
43	289.0536	2.69	6.78	0	43	1
47	287.0760	2.84	6.05	0	47	1
48	359.0454	2.57	7.25	0	48	1
49	286.0742	2.11	6.56	0	49	1
62	361.0425	2.57	7.89	0	62	1

